I. General Information

CAS Number: Free 3,3' Dichlorobenzidine (CAS NO.: 91-94-1)

Name:

II. Physical-Chemical Data

A1. Melting Point

Test Substance

Test substance: DCB

Remarks:

Method

Method: Measured

Remarks:

Results

Melting point value: 132 °C

Remarks:

References

Merck. 1989. The Merck Index: An Encyclopedia of Chemicals, Drugs, and Biologicals. 11th ed.Rahway, NJ: Merck and Company, Inc., 482.

Other

Data is from a reputable reference.

B. Boiling Point

Test Substance

Test substance: DCB

Remarks:

Method

Method:

Remarks:

Results

Boiling point value: 402 °C

Remarks:

References

Hazardous Substance Data Bank, 1996, National Library of Medicine, National Toxicology Information Program, Bethesda, MD. Cited by ATSDR

Other

Data reported from reputable sources

C1. Vapor Pressure

Test Substance

Test substance: DCB

Remarks:

Method

Method: Estimate
Remarks:

Results

Vapor pressure value: .45
Temperature:

Remarks:

References

MPBPWIN v 1.40 in EPIWIN v 3.10, Syracuse Research Corporation, Syracuse, New York

Other

D. Partition Coefficient

Test Substance

Test substance: DCB

Remarks:

Method

Method: actual analysis
Remarks:

Results

Value: 3.2
Remarks:

References

Log Kow partition coefficient reported by Mabey et al. Aquatic Fate process data for organic priority pollutants, EPA Study No. 440/4-81-014, See Also Fate of 3,3' Dichlorobenzidine in Aquatic Environments, EPA Study No. 600/3-78-068, and ATSDR Toxicological Profile DCB

Other

E. Water Solubility

Test Substance

Test substance: DCB

Remarks:

Method

Method: The Solubility of DCB.2HCL in aqueous buffers of pH 4.6-8.9 at 22 degrees centigrade was determined spectrophotometrically from a knowledge of the extinction coefficients of its UV absorption maxima. The UV spectra of these solutions were recorded, and the values derived from at least two separately weighed methanol solutions, and from 4 to 6 spectral determinations.

Remarks:

Results

Value: 2-4 %
Temperature: 22 °C
Description: Slightly Soluble
Remarks:

References

Sikka HC, Appleton HT, Banerjee S. 1978. Fate of 3,3'-dichlorobenzidine in aquatic environments, U.S. Environmental Protection Agency. EPA-600/3-78-068.

Other

Environmental Fate Endpoints

A. Photodegradation

Test Substance

Test substance: DCB

Remarks:

Method

Method:

Test type: Water\sunlight and artificial laboratory lighting

Remarks:

Results

Temperature:

Degradation Rate

5-30 minutes in laboratory lighting

: Half-life

Ozone reaction: 90 seconds in natural light

Remarks:

Conclusions

References

Sikka HC, Appleton HT, Banerjee S. 1978. Fate of 3,3'-dichlorobenzidine in aquatic environments, U.S. Environmental Protection Agency. EPA-600/3-78-068.

Other

B. Stability in Water

Test Substance

Test substance:	DCB
Remarks:	

Method

Method:	estimates based on surrogate substances
Test type:	
GLP:	
Remarks:	

Results

Half-life:	½ life 100 days
Percent hydrolyzed in 5 days (120 hs) at 50 °C :	Hydrolysis rate 0/Mole per hour (Mabey et al.)
Remarks:	Under the conditions of an anaerobic biodegradation test with a similar compound (biazoaryl pigment), no hydrolysis was observed within 56 days

Conclusions

Data Quality

Remarks:

References

Other

Callahan MA, Slimak, Gabel NW, et al. 1979. Water-related environmental fate of 129 priority pollutants. V. II. U.S. Environmental Protection Agency. EPA-440/4-79-029b. See also, Mabey WR, Smith JH, Pod RT, et al. 1982. Aquatic fate process data for organic priority pollutants. Washington, DC: Office of Water Regulations and Standards, U.S. Environmental Protection Agency. EPA 440/4-81-014. PB87-169090.

C. Biodegradation

Test Substance

Test substance: DCB

Remarks:

Method

Method: EPA Microbial Degradation

Test type: Microbial degredation in surface waters and activated sludge

GLP:

Year:

Remarks: Two separate studies one 28 days the other 30 days the second used C^{14} labeling, Degradation was negligible in both studies. The third study used activated sludge

Results

Results:

Remarks: negligible biodegradation observed in all three studies

Conclusions

Data Quality

Remarks: Data is very well documented, readily available and of very high quality.

References

Other

Sikka HC, Appleton HT, Banerjee S. 1978. Fate of 3,3'-dichlorobenzidine in aquatic environments, U.S. Environmental Protection Agency. EPA-600/3-78-068.

D. Transport between Environmental Compartments (Fugacity)

Test Substance

Test substance: DCB

Remarks:

Method

Test type: Estimation

Model used: Level III Fugacity Model; EPIWIN:EQC from Syracuse Research Corporation

Remarks:

Results

Model data and results:

Distribution (%)	
Air	1.13×10^{-5}
Water	47.5
Soil	52.4
Sediment	.095

Remarks:

Conclusions

Since no experimental values were available the physical chemical values utilized in this model were default parameters from within EPIWIN.

References

Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210.

Other

The Level III model incorporated into EPIWIN is a Syracuse Research Corporation adaptation of the methodology described by Mackay *et al.* 1996; *Environ. Toxicol. Chem.* **15(9)**, 1618-1626 and 1627-1637.

V. Ecotoxicity

A. Acute Toxicity to Fish

Test Substance

Test substance:	DCB
Remarks:	

Method

Method:	EPA Bioconcentration
Test type:	Static
GLP:	N/A
Year:	1978
Species/strain:	Bluegill
Analytical monitoring:	Exposure solutions,
Exposure period:	96-Hour and 120 -Hour
Remarks:	Fish were exposed to 2 nominal concentrations(.5 and 2 mg/L), Glass containers were stored away from any light source

Results

Nominal concentration:	
Measured concentration:	
Endpoint value:	
Biological observations:	
Statistical methods:	
Remarks:	Significant mortality observed, surviving fish were severly intoxicated and would have succembed if the study contiued beyond 120 hours

Conclusions

Test substance is toxic to fish

Sikka et al. (1978) reported a 48-hour LC100 value for bluegill sunfish (Lepomis macrochirus) of 2 mg/litre 50% mortality was observed following exposure to 3,3'-dichlorobenzidine at 0.5 mg/litre for 96-120 hours. Based on quantitative structure-activity relationships, 96-hour LC50 values for fathead minnow (Pimephales promelas), rainbow trout (Oncorhynchus mykiss), and golden orfe (Leuciscus idus melanotus) have been estimated to be, 3 mg/litre, and 1.5 mg/litre, respectively (Government of Canada, 1993).

Data Quality

Reliability:

Remarks:

Data is very well documented, readily available and of very high quality.

References

Sikka HC, Appleton HT, Banerjee S. 1978. Fate of 3,3'-dichlorobenzidine in aquatic environments, U.S. Environmental Protection Agency. EPA-600/3-78-068., See also, Appleton et al. Accumulation , elimination, and metabolism of dichlorobenzidine in the bluegill sunfish, Environ. Sci. Technol. Vol. 14, pp.50-54 (1980)

Other

B. Acute Toxicity to Aquatic InvertebratesTest

Substance

Test substance:

Remarks: DCB

Method

Method:
Test type:
GLP:
Year: estimate
Species/strain: Static
Analytical monitoring:
Exposure period: Daphnid (*Daphnia magna*)
Remarks: Temperature, pH and dissolved oxygen
48 Hours

Results

Nominal concentration:
Measured concentration:
Endpoint value:
Reproduction
Biological observations: LC 50 6664.850 mg/L
Statistical methods:
Remarks:

Conclusions

Data Quality

Reliability:
Remarks:

References

Other

Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210. The Level III model incorporated into EPIWIN is a Syracuse Research Corporation adaptation of the methodology described by Mackay *et al.* 1996; *Environ. Toxicol. Chem.* **15(9)**, 1618-1626 and 1627-1637.

Due to characteristics in water and light, there are very few data on the acute toxicity of 3,3'-dichlorobenzidine to aquatic organisms. An IC50 of 0.06 mg/litre was reported for bacteria in the Microtox assay (Dutka & Kwan, 1981). ;

B2. Chronic Toxicity to Aquatic InvertebratesTest

Substance

Test substance:

Remarks: DCB

Method

Method:
Test type:
GLP:
Year: estimation
Species/strain:
Analytical monitoring:
Exposure period:
Remarks: Daphnid

16 days

Results

Nominal concentration:
Measured concentration:
Endpoint value:
Reproduction
Biological observations:
Statistical methods: EC 50 - 173.496 mg/L
Remarks:

Conclusions

Data Quality

Reliability:
Remarks:

References

Other

Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210.

C. **Toxicity to Aquatic Plants**

Test Substance

Test substance: DCB

Remarks:

Method

Method: Estimation
Test type:
GLP:
Year:
Species/strain: Green Algae
Endpoint basis:
Exposure period: 96 Hours
Analytical procedures:
Remarks:

Results

Nominal concentration:
Measured concentration:
Endpoint value: EC_{50} 3811.012 mg/L ChV 155.593 mg/L
NOEC:
Biological observations:
Was control response
:satisfactory
Statistical Methods: ANOVA
Remarks:

Conclusions

Data Quality

Reliability:
Remarks:

References

Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210.

Other

V. Toxicological Data

A. Acute Toxicity

Test Substance

Test substance:	DCB
Remarks:	Purity was unknown

Method

Method:	Acute lethality; Other
Test type:	LD_{50} estimate
GLP:	No (Pre-GLP)
Year:	1974
Species/strain:	Rat/unknown
Route of exposure:	Oral gavage
Dose levels:	Unknown
Remarks:	

Results

Value:	LD_{50} = > 7070/3820 mg/kg.
Deaths at each dose:	
Remarks:	

Conclusions

Data Quality

Reliability:	Reliable with restrictions
Remarks:	The study was conducted quite some time ago and hence many study details are missing from the report and not available. However, basic data are given and results are consistent with other data for pigments of this class.

References

Gerarde HW, Gerarde DF. 1974. Industrial experience with 3,3'-dichlorobenzidine: An epidemiological study of a chemical manufacturing plant. J Occup Med 16(5):322-344.

Other

Repeated Dose Toxicity Test

Substance

Test substance:	DCB
Remarks:	

Method

Method:	repeated dose
Test type:	Sub acute
GLP:	no
Year:	1979
Species/strain:	Mouse Female
Route of exposure:	Ingestion
Duration of test:	6 or 12 months
Exposure levels:	54, 157, 4
Sex:	female
Exposure period:	6 an 12 months
Post-exposure observation period:	
Remarks:	

Results

NOAEL (NOEL):	<54mg/m3 Mortality: none Hepatomas in 8/8 at 6 months and in18/18 at 12 months

Conclusions Test substance may be considered toxic

Data Quality

Reliability:	Reliable without restriction
Remarks:	

References:

Osanai H. 1976. [An experimental study on hepatoma caused by aromatic amines.] Rodo Kagaku 52: 179-201. (Japanese)

Other

Repeated Dose Toxicity Test

Substance

Test substance:	DCB
Remarks:	

Method

Method:	repeated dose
Test type:	Chronic
GLP:	no
Year:	1978
Species/strain:	Dog, Beagle
Route of exposure:	Gavage
Duration of test:	6 weeks and 7.1 years
Exposure levels:	
Sex:	Male and female
Exposure period:	
Post-exposure observation period:	
Remarks:	

Results

LOAEL:	10.4 mg/kg/day heptacellular carcinomas in 4/6 papillary transitional cell carcinomas of urinary bladder in 5/6

Conclusions

Data Quality

Reliability:	Reliable without restriction
Remarks:	

References:

Stula EF, Barnes JR, Sherman H, et al. 1978. Liver and urinary bladder tumors in dogs from 3,3'-dichlorobenzidine. J Environ Pathol Toxicol 1(4):475-490.

Other

C. **Genetic Toxicity - Mutation**

Test Substance

Test substances:	DCB
Remarks:	

Method

Method:	In Vitro Mutagenicity
Test type:	Ames
GLP:	Unknown
Year:	1986
Species/strain:	Hamster liver / Salmonella typhimurium
Metabolic activation:	Yes, S9
Concentration tested:	
Remarks:	

Results

Result:	Positive
Cytotoxic concentration:	
Precipitation concentration:	Negative
Genotoxic effects	Negative
With activation:	
Without activation:	
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability:	Published study reliable without restriction
Remarks:	

References

Savard, S. and Josephy, PD. Synthesis and Mutagenicity of 3,3' Dihalogenated Benzidines, Carcinogenesis, Vol.7 pp.1239-1241, (1986) (cited in ATSDR)

D. Genetic Toxicity – Chromosomal Aberrations

Test Substance

Test substance:	DCB
Remarks:	Chromosomal aberation test CHO cells

Method no

Method:	
Test type:	Mouse Bone Marrow (Male and Female) Mouse Fetal Liver
GLP:	
Year:	1987
Species/strain:	
Exposure period:	
Remarks:	

Results

Result:	Negative femal bone marrow, positive male bone marrow and fetal liver
Genotoxic effects:	
Concentration tested	
Statistical methods:	
Remarks:	

Conclusions

Data Quality

Reliability:	Reliable without restriction
Remarks:	

References

Cihak R., Vontorvoka M. "Benzidine and 3,3' Dichlorobenzidine Induce Micronuclei inthe Bone Marrow and the FetalLiver of Mice after Gavage", Mtugenesis Vol.2 pp. 267-269 (1987) See also
Iba MM, Ghosal A, Poyer JL, et al. 1991. In vivo spin-trapping of the radical metabolites of 3,3,'dichlorobenzidine and related compounds in the rat. Progress in Pharmacology and Clinical Pharmacology 8(3):255-266.
Ashby J, Mohammed R. 1988. UDS activity in the rat liver of the human carcinogens benzidine and 4-aminobiphenyl and the rodent carcinogens 3,3'-dichlorobenzidine and Direct Black 38. Mutagenesis 3(1):69-7 1.

Other

E. Developmental Toxicity

Test Substance

Test substance: DCB

Remarks:

Method

Method:

GLP: See Repeated Dose Studies

Year:

Species/strain:

Sex:

Route of exposure:

Exposure levels:

Actual doses received:

Exposure period:

Duration of test:

Remarks:

Results

Maternal toxicity

NOEL:

NOEL for teratogenicity:

NOEL for fetotoxicity:

Parental toxic responses:

Fetal toxic responses dose:

Statistical Methods:

Remarks: Studies in which pregnant mice were exposed to the chemical, the kidneys of their babies did not develop properly.

Conclusions

Data Quality

Reliability: Golub et al. Oncogenic Action of Some Nitrogen Compounds on the Progeny of Experimental Mice" Bull. Exp. Biol. Med. Vol.78 pp. 1402-1404 (1975) (Russian)

Remarks:

References

Other

F. Toxicity to Reproduction

Test Substance

Test substance: DCB
Remarks:

Method

Method:
GLP:
Year:
Species/strain:
Sex:
Route of exposure:
Exposure levels:

Exposure period:

Duration of test:
Remarks:

Results

Maternal toxicity NOEL:
Parental toxic responses:
Fetal toxic responses dose:
Statistical Methods:
Remarks:

Conclusions

Data Quality

Reliability:
Remarks:

References

Other

Acute toxicity

Test substance: DCB

Remarks:

Method

Method:	Irritation to the rabbit eye
Test type:	eye irritation
GLP:	yes
Year:	1974
Species/strain:	rabbit, New Zealand albino (chbb:Nzw)
Route of exposure:	
Dose levels:	
Remarks:	

Results

Value:	Cornea .55, iris .33 conjunctive (redness) 2.44) (Chemosis .88)
Deaths at each dose:	
Remarks:	observation times ?? Reversibility within

Conclusions NOAEL 100 mg

Data Quality

Reliability:	reliable without restriction
Remarks:	

References Gerarde HW, Gerarde DF. 1974. Industrial experience with 3,3'-dichlorobenzidine: An epidemiological study of a chemical manufacturing plant. J Occup Med 16(5):322-344.

Other

Acute toxicity

Test substance:	DCB
Remarks:	

Method

Method:	Skin irritation to the rabbit
Test type:	Skin irritation intradermal installation SEMIOCCLUSIVE
GLP:	N/A
Year:	1974
Species/strain:	rabbit New Zealand albino
Route of exposure:	
Dose levels:	700 mg/kg
Remarks:	

Results

Value:	not irritating
Deaths at each dose:	
Remarks:	

Conclusions not irritating

Data Quality

Reliability:	Valid without restriction
Remarks:	

Reference

Gerarde HW, Gerarde DF. 1974. Industrial experience with 3,3'-dichlorobenzidine: An epidemiological study of a chemical manufacturing plant. J Occup Med 16(5):322-344.

Chronic Dose Toxicity Test Substance

Test substance: DCB

Method

Method: Chronic Toxicity
Test type: Repeated oral dose
GLP: unknown
Year: See references below
Species/strain: Rat,dogs, hamsters,mice
Route of exposure: Oral gavage
Duration of test: 104 Weeks
Exposure levels: 1 to 7 years
Sex: Male and Female
Exposure period:
Post-exposure observation period:
Remarks:

Results

NOAEL (NOEL): Vary by study

Conclusions Neoplasia in a variety of target organs and a variety of species

Data Quality

Reliability: published data, valid without restriction
Remarks:

References

blastomogenic agent] Vop Onkol 5(5):524-533.
experimental study on hepatoma caused by aromatic
(Japanese) Sellakumar AR, Montesano R,
carcinogenicity in hamsters. Division of Oncology. The
Eppley Inst. for Res in Cancer, University of Nebraska, Omaha.
JR, Sherman H, et al. 1978. Liver and urinary bladder tumors in
dichlorobenzidine. J Environ Pathol Toxicol 1(4):475-490, Ito N,
al. 1983. Modifying factors in urinary bladder carcinogenesis.
222.

Pliss GB. 1959. [Dichlorobenzidine as a
(Russian), Osanai H. 1976. [An
amines.] Rodo Kagaku 52: 179-201.
Saffiotti U. 1969. Aromatic amines
Chicago Medical School and
[abstract] Stula EF, Barnes
dogs from 3,3'-
Fukushima S, Shirai T, et
Environ Health Perspect 49:217-

Other

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